Random sampling locations for comparing a mean with a fixed threshold (parametric)

Summary

This report summarizes the sampling design, associated statistical assumptions, as well as general guidelines for conducting post-sampling data analysis. Sampling plan components presented here include how many sampling locations to choose and where within the sampling area to collect those samples. The type of medium to sample (i.e., soil, groundwater, etc.) and how to analyze the samples (in-situ, fixed laboratory, etc.) are addressed in other sections of the sampling plan.

The following table summarizes the sampling design. A figure that shows sampling locations in the field and a table that lists sampling location coordinates are also provided below.

SUMMARY OF SAMPLING DESIGN	
Primary Objective of Design	Compare a site mean to a fixed threshold
Type of Sampling Design	Parametric
Sample Placement (Location) in the Field	Simple random sampling
Working (Null) Hypothesis	The mean value at the site exceeds the threshold
Formula for calculating number of sampling locations	Student's t-test
Calculated total number of samples	23
Number of samples on map [a]	41
Number of selected sample areas [b]	2
Specified sampling area [c]	188054.34 m^2
Total cost of sampling [d]	$12,500.00

[a] This number may differ from the calculated number because of 1) grid edge effects, 2) adding judgment samples, or 3) selecting or unselecting sample areas.
[b] The number of selected sample areas is the number of colored areas on the map of the site. These sample areas contain the locations where samples are collected.
[c] The sampling area is the total surface area of the selected colored sample areas on the map of the site.
[d] Including measurement analyses and fixed overhead costs. See the Cost of Sampling section for an explanation of the costs presented here.

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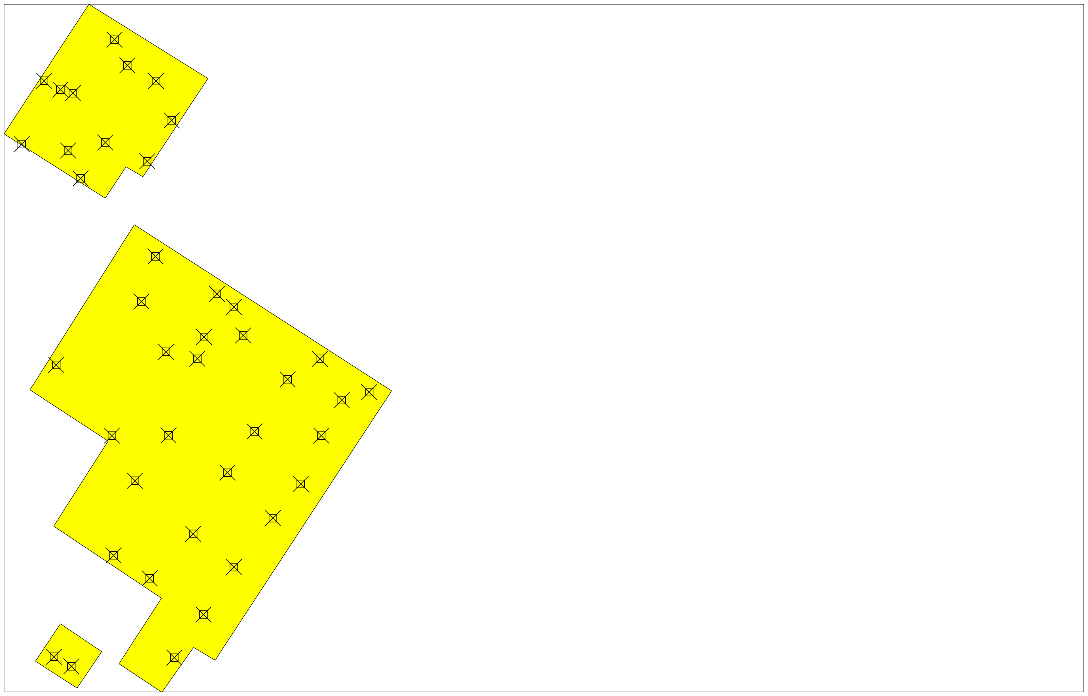


Area: Area 1					
X Coord	Y Coord	Label	Value	Type	Historical
679133.4290	3083306.3130	J-01S	3010	Manual	T
679104.2450	3083223.2620	J-02S	820	Manual	T
679155.0740	3083294.6960	J-03S	659.5	Manual	T
679171.2970	3083289.7960	J-04S	786	Manual	T
679225.8560	3083359.9740	J-05S	1250	Manual	T
679164.8060	3083214.7100	J-06S	609	Manual	T
679242.7260	3083326.5280	J-07S	2900	Manual	T
679181.2750	3083178.2880	J-08S	5020	Manual	T
679213.7730	3083224.9730	J-09S	5460	Manual	T
679280.5440	3083305.6810	J-10S	1670	Manual	T
679268.7700	3083200.3260	J-11S	14300	Manual	T
679301.1600	3083254.0340	J-12S	3550	Manual	T

Area: Area 3					
X Coord	Y Coord	Label	Value	Type	Historical
679149.4920	3082933.0980	J-13S	2590	Manual	T
679279.6830	3083075.4290	J-14S	2710	Manual	T
679261.0980	3083016.3510	J-15S	1440	Manual	T
679222.6340	3082840.1720	J-16S	3680	Manual	T
679293.5600	3082950.4980	J-17S	7070	Manual	T
679360.5700	3083026.4980	J-18S	3030	Manual	T
679343.5810	3082969.5980	J-19S	4375	Manual	T

679382.8640	3083009.1130	J-20S	4570	Manual	T
679335.0020	3082941.1720	J-21S	4470	Manual	T
679252.7130	3082781.0290	J-22S	5620	Manual	T
679297.0010	3082840.6970	J-23S	8090	Manual	T
679394.8070	3082971.8300	J-24S	2110	Manual	T
679146.6460	3082549.7640	J-25S	1105	Manual	T
679224.5850	3082683.1400	J-26S	2540.05	Manual	T
679169.0760	3082537.3510	J-27S	2550	Manual	T
679272.0040	3082652.6750	J-28S	5510	Manual	T
679329.4380	3082711.0960	J-29S	12200	Manual	T
679374.4420	3082791.3300	J-30S	14400	Manual	T
679410.1490	3082845.8460	J-31S	15650	Manual	T
679453.4760	3082914.1150	J-32S	14200	Manual	T
679495.8840	3082940.9730	J-33S	2600	Manual	T
679304.6530	3082548.6880	J-34S	25400	Manual	T
679342.7410	3082605.3190	J-35S	5130	Manual	T
679382.8900	3082667.5270	J-36S	7830	Manual	T
679433.9450	3082731.6820	J-37S	6190	Manual	T
679470.3570	3082776.7350	J-38S	9900	Manual	T
679497.3310	3082840.3960	J-39S	5110	Manual	T
679524.3310	3082886.8990	J-40S	9850	Manual	T
679560.6070	3082897.2580	J-41S	4830	Manual	T

Primary Sampling Objective
The primary purpose of sampling at this site is to compare a mean value of a site with a fixed threshold. The working hypothesis (or 'null' hypothesis) is that the mean value at the site is equal to or exceeds the threshold. The alternative hypothesis is that the mean value is less than the threshold. VSP calculates the number of samples required to reject the null hypothesis in favor of the alternative hypothesis, given a selected sampling approach and inputs to the associated equation.

Selected Sampling Approach
A parametric random sampling approach was used to determine the number of samples and to specify sampling locations. A parametric formula was chosen because the conceptual model and historical information (e.g., historical data from this site or a very similar site) indicate that parametric assumptions are reasonable. These assumptions will be examined in post-sampling data analysis.

Both parametric and non-parametric approaches rely on assumptions about the population. However, non-parametric approaches typically require fewer assumptions and allow for more uncertainty about the statistical distribution of values at the site. The trade-off is that if the parametric assumptions are valid, the required number of samples is usually less than the number of samples required by non-parametric approaches.

Locating the sample points randomly provides data that are separated by many distances, whereas systematic samples are all equidistant apart. Therefore, random sampling provides more information about the spatial structure of the potential contamination than systematic sampling does. As with systematic sampling, random sampling also provides information regarding the mean value, but there is the possibility that areas of the site will not be represented with the same frequency as if uniform grid sampling were performed.

Number of Total Samples: Calculation Equation and Inputs
The equation used to calculate the number of samples is based on a Student's t-test. For this site, the null hypothesis is rejected in favor of the alternative hypothesis if the sample mean is sufficiently smaller than the threshold. The number of

samples to collect is calculated so that 1) there will be a high probability ($1-\beta$) of rejecting the null hypothesis if the alternative hypothesis is true and 2) a low probability (α) of rejecting the null hypothesis if the null hypothesis is true.

The formula used to calculate the number of samples is:

$$n = \frac{S^2}{\Delta^2}\left(Z_{1-\alpha} + Z_{1-\beta}\right)^2 + 0.5Z_{1-\alpha}^2$$

where

n	is the number of samples,
S	is the estimated standard deviation of the measured values including analytical error,
Δ	is the width of the gray region,
α	is the acceptable probability of incorrectly concluding the site mean is less than the threshold,
β	is the acceptable probability of incorrectly concluding the site mean exceeds the threshold,
$Z_{1-\alpha}$	is the value of the standard normal distribution such that the proportion of the distribution less than $Z_{1-\alpha}$ is $1-\alpha$,
$Z_{1-\beta}$	is the value of the standard normal distribution such that the proportion of the distribution less than $Z_{1-\beta}$ is $1-\beta$.

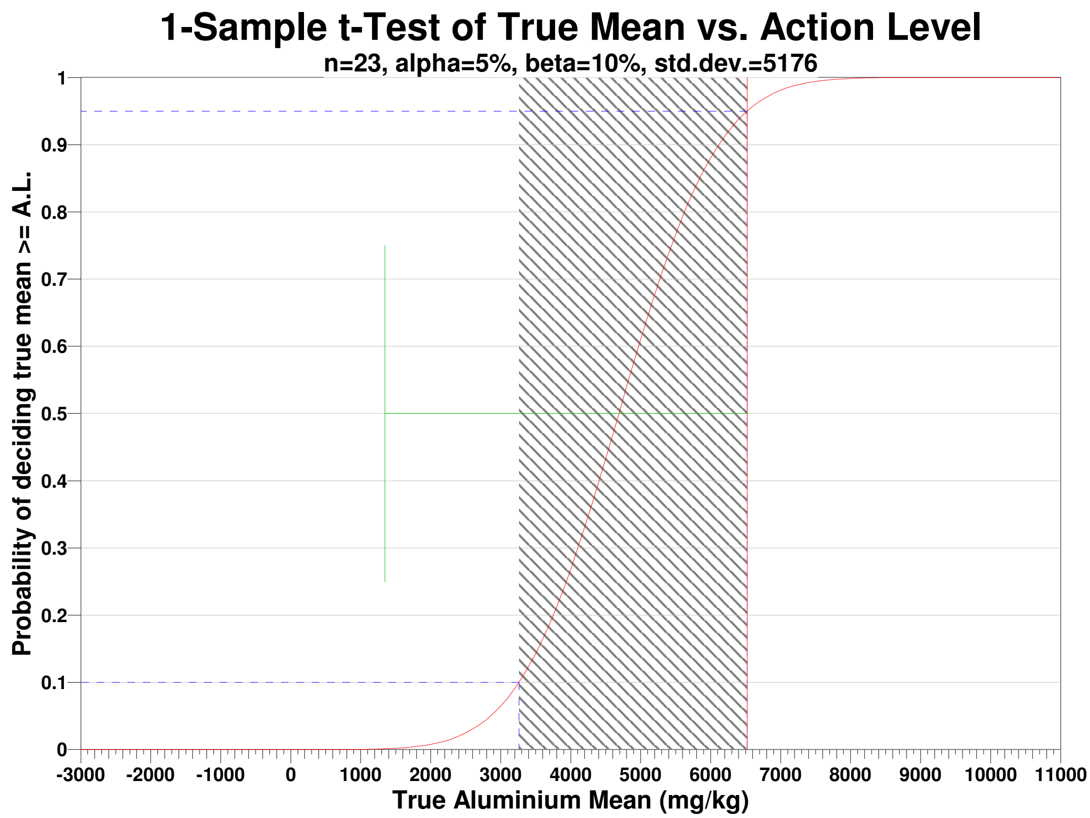
The values of these inputs that result in the calculated number of sampling locations are:

Analyte	**n**	**Parameter**					
		S	**Δ**	**α**	**β**	**$Z_{1-\alpha}$** [a]	**$Z_{1-\beta}$** [b]
Aluminium	23	5176 mg/kg	3261 mg/kg	0.05	0.1	1.64485	1.28155

[a] This value is automatically calculated by VSP based upon the user defined value of α.
[b] This value is automatically calculated by VSP based upon the user defined value of β.

The following figure is a performance goal diagram, described in EPA's QA/G-4 guidance (EPA, 2000). It shows the probability of concluding the sample area is dirty on the vertical axis versus a range of possible true mean values for the site on the horizontal axis. This graph contains all of the inputs to the number of samples equation and pictorially represents the calculation.

The red vertical line is shown at the threshold (action limit) on the horizontal axis. The width of the gray shaded area is equal to Δ; the upper horizontal dashed blue line is positioned at $1-\alpha$ on the vertical axis; the lower horizontal dashed blue line is positioned at β on the vertical axis. The vertical green line is positioned at one standard deviation below the threshold. The shape of the red curve corresponds to the estimates of variability. The calculated number of samples results in the curve that passes through the lower bound of Δ at β and the upper bound of Δ at $1-\alpha$. If any of the inputs change, the number of samples that result in the correct curve changes.



Statistical Assumptions

The assumptions associated with the formulas for computing the number of samples are:

1. the sample mean is normally distributed (this happens if the data are roughly symmetric or the sample size is more than 30; for extremely skewed data sets, additional samples may be required for the sample mean to be normally distributed),
2. the variance estimate, S^2, is reasonable and representative of the population being sampled,
3. the population values are not spatially or temporally correlated, and
4. the sampling locations will be selected randomly.

The first three assumptions will be assessed in a post data collection analysis. The last assumption is valid because the sample locations were selected using a random process.

Sensitivity Analysis

The sensitivity of the calculation of number of samples was explored by varying the standard deviation, lower bound of gray region (% of action level), beta (%), probability of mistakenly concluding that μ > action level and alpha (%), probability of mistakenly concluding that μ < action level. The following table shows the results of this analysis.

Number of Samples							
AL=6521		**α=5**		**α=10**		**α=15**	
		s=10352	**s=5176**	**s=10352**	**s=5176**	**s=10352**	**s=5176**
LBGR=90	**β=5**	2729	684	2160	541	1813	454
	β=10	2160	541	1657	415	1355	340
	β=15	1814	455	1355	340	1084	272
LBGR=80	**β=5**	684	172	541	136	454	114
	β=10	541	137	415	105	340	86
	β=15	455	115	340	86	272	69
LBGR=70	**β=5**	305	78	241	61	202	51

	β=10	242	62	185	47	151	39
	β=15	203	52	152	39	121	31

s = Standard Deviation
LBGR = Lower Bound of Gray Region (% of Action Level)
β = Beta (%), Probability of mistakenly concluding that μ > action level
α = Alpha (%), Probability of mistakenly concluding that μ < action level
AL = Action Level (Threshold)

Cost of Sampling
The total cost of the completed sampling program depends on several cost inputs, some of which are fixed, and others that are based on the number of samples collected and measured. Based on the numbers of samples determined above, the estimated total cost of sampling and analysis at this site is $12,500.00, which averages out to a per sample cost of $543.48. The following table summarizes the inputs and resulting cost estimates.

COST INFORMATION			
Cost Details	**Per Analysis**	**Per Sample**	**23 Samples**
Field collection costs		$100.00	$2,300.00
Analytical costs	$400.00	$400.00	$9,200.00
Sum of Field & Analytical costs		**$500.00**	**$11,500.00**
Fixed planning and validation costs			$1,000.00
Total cost			**$12,500.00**

Data Analysis for Aluminium
The following data points were entered by the user for analysis.

Aluminium (mg/kg)										
Rank	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
0	609	659.5	786	820	1105	1250	1440	1670	2110	2540
10	2550	2590	2600	2710	2900	3010	3030	3550	3680	4375
20	4470	4570	4830	5020	5110	5130	5460	5510	5620	6190
30	7070	7830	8090	9850	9900	1.22e+004	1.42e+004	1.43e+004	1.44e+004	1.565e+004
40	2.54e+004									

SUMMARY STATISTICS for Aluminium	
n	41
Min	609
Max	25400
Range	24791
Mean	5726.5
Median	4470
Variance	2.6787e+007
StdDev	5175.7
Std Error	808.3
Skewness	1.857

Interquartile Range				4905				
Percentiles								
1%	**5%**	**10%**	**25%**	**50%**	**75%**	**90%**	**95%**	**99%**
609	672.1	877	2545	4470	7450	1.428e+004	1.552e+004	2.54e+004

Outlier Test
Rosner's test for multiple outliers was performed to test whether the most extreme value is a statistical outlier. The test was conducted at the 5% significance level.

Data should not be excluded from analysis solely on the basis of the results of this or any other statistical test. If any values are flagged as possible outliers, further investigation is recommended to determine whether there is a plausible explanation that justifies removing or replacing them.

In using Rosner's test to detect up to 1 outlier, a test statistic R_1 is calculated, and compared with a critical value C_1 to test the hypothesis that there is one outlier in the data.

ROSNER'S OUTLIER TEST for Aluminium			
k	**Test Statistic R_k**	**5% Critical Value C_k**	**Significant?**
1	3.801	3.05	Yes

The test statistic 3.801 exceeded the corresponding critical value, therefore that test is significant and we conclude that the most extreme value is an outlier at the 5% significance level.

SUSPECTED OUTLIERS for Aluminium	
1	25400

A normal distribution test indicated that the data do not appear to be normally distributed, so further investigation is recommended before using the results of this test. Because Rosner's test can be used only when the data without the suspected outlier are approximately normally distributed, a Shapiro-Wilk test for normality was performed at a 5% significance level.

NORMAL DISTRIBUTION TEST (excluding outliers)	
Shapiro-Wilk Test Statistic	0.8538
Shapiro-Wilk 5% Critical Value	0.94

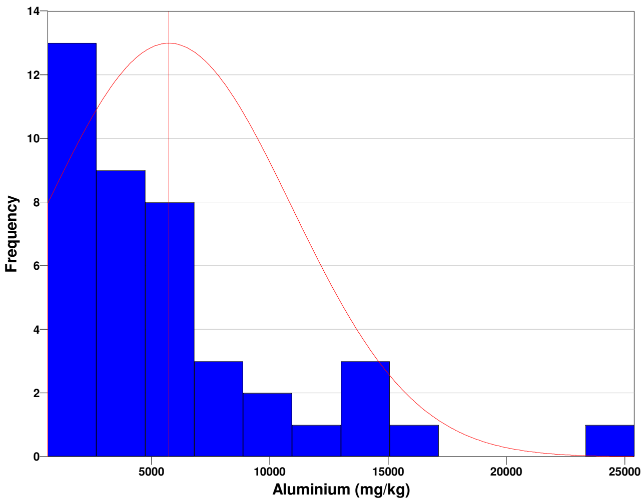
The calculated Shapiro-Wilk test statistic is less than the 5% Shapiro-Wilk critical value, so the test rejects the hypothesis that the data are normal and concludes that the data, excluding the most extreme value, do not appear to follow a normal distribution at the 5% level of significance. Rosner's test may not be appropriate if the assumption of normally distributed data is not justified for this data set. Examine the Q-Q plot displayed below to further assess the normality of the data.

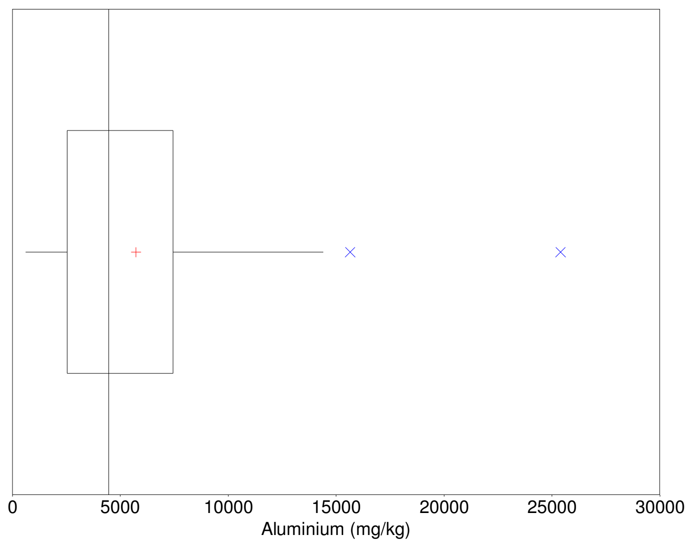
Data Plots for Aluminium
Graphical displays of the data are shown below.

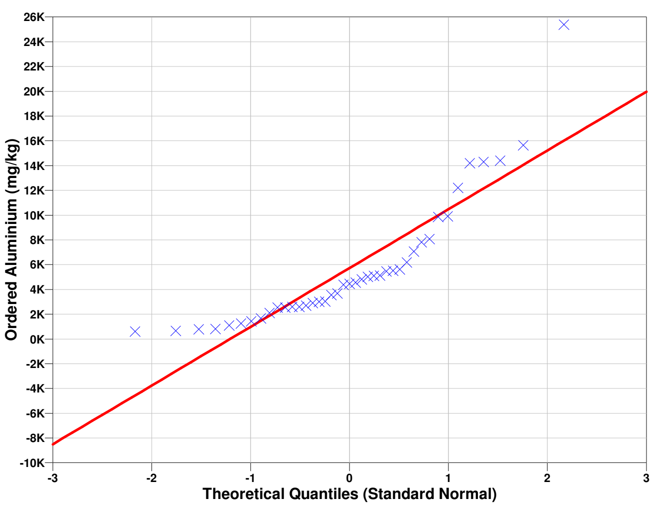
The Histogram is a plot of the fraction of the n observed data that fall within specified data “bins.” A histogram is generated by dividing the x axis (range of the observed data values) into "bins" and displaying the number of data in each bin as the height of a bar for the bin. The area of the bar is the fraction of the n data values that lie within the bin. The sum of the fractions for all bins equals one. A histogram is used to assess how the n data are distributed (spread) over their range of values. If the histogram is more or less symmetric and bell shaped, then the data may be normally distributed.

The Box and Whiskers plot is composed of a central box divided by a line, and with two lines extending out from the box, called the "whiskers". The line through the box is drawn at the median of the n data observed. The two ends of the box represent the 25^{th} and 75^{th} percentiles of the n data values, which are also called the lower and upper quartiles, respectively, of the data set. The sample mean (mean of the n data) is shown as a "+" sign. The upper whisker extends to the largest data value that is less than the upper quartile plus 1.5 times the interquartile range (upper quartile minus the lower quartile). The lower whisker extends to the smallest data value that is greater than the lower quartile minus 1.5 times the interquartile range. Extreme data values (greater or smaller than the ends of the whiskers) are plotted individually as blue Xs. A Box and Whiskers plot is used to assess the symmetry of the distribution of the data set. If the distribution is symmetrical, the box is divided into two equal halves by the median, the whiskers will be the same length, and the number of extreme data points will be distributed equally on either end of the plot.

The Q-Q plot graphs the quantiles of a set of n data against the quantiles of a specific distribution. We show here only the Q-Q plot for an assumed normal distribution. The p^{th} quantile of a distribution of data is the data value, x_p, for which a fraction p of the distribution is less than x_p. If the data plotted on the normal distribution Q-Q plot closely follow a straight line, even at the ends of the line, then the data may be assumed to be normally distributed. If the data points deviate substantially from a linear line, then the data are not normally distributed.







For more information on these plots consult Guidance for Data Quality Assessment, EPA QA/G-9, pgs 2.3-1 through 2.3-12. (http://www.epa.gov/quality/qa-docs.html).

Tests for Aluminium
A goodness-of-fit test was performed to test whether the data set had been drawn from an underlying normal distribution. The Shapiro-Wilk (SW) test was used to test the null hypothesis that the data are normally distributed. The test was conducted at the 5% significance level, i.e., the probability the test incorrectly rejects the null hypothesis was set at 0.05.

NORMAL DISTRIBUTION TEST	
Shapiro-Wilk Test Statistic	0.8145
Shapiro-Wilk 5% Critical Value	0.941

The calculated SW test statistic is less than the 5% Shapiro-Wilk critical value, so we can reject the hypothesis that the data are normal, or in other words the data do not appear to follow a normal distribution at the 5% level of significance. The Q-Q plot displayed above should be used to further assess the normality of the data.

Upper Confidence Limit on the True Mean
Two methods were used to compute the upper confidence limit (UCL) on the mean. The first is a parametric method that assumes a normal distribution. The second is the Chebyshev method, which requires no distributional assumption.

UCLs ON THE MEAN	
95% Parametric UCL	7088
95% Non-Parametric (Chebyshev) UCL	9250

Because the data do not appear to be normally distributed according to the goodness-of-fit test performed above, the non-parametric UCL (9250) may be a more accurate upper confidence limit on the true mean.

One-Sample t-Test
A one-sample t-test was performed to compare the sample mean to the action level. The null hypothesis used is that the true mean equals or exceeds the action level (AL). The t-test was conducted at the 5% significance level. The sample value *t* was computed using the following equation:

$$t = \frac{\bar{x} - AL}{SE}$$

where
x is the sample mean of the n=41 data,
AL is the action level or threshold (6521),
SE is the standard error = (standard deviation) / (square root of n).

This *t* was then compared with the critical value $t_{0.95}$, where $t_{0.95}$ is the value of the t distribution with n-1=40 degrees of freedom for which the proportion of the distribution to the left of $t_{0.95}$ is 0.95. The null hypothesis will be rejected if $t < -t_{0.95}$.

ONE-SAMPLE t-TEST		
t-statistic	**Critical Value $t_{0.95}$**	**Null Hypothesis**
-0.98298	1.6839	Cannot Reject

The test did not reject the null hypothesis that the mean value at the site exceeds the threshold, therefore conclude the true mean exceeds the threshold.

Because the data do not appear to be normally distributed, the MARSSIM Sign Test might be preferred over the One Sample t-Test. The following table represents the results of the MARSSIM Sign Test using the current data:

MARSSIM Sign Test		
Test Statistic (S+)	**95% Critical Value**	**Null Hypothesis**
30	26	Reject